

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042018\
 Data File : BF104684.D
 Acq On : 20 Apr 2018 19:40
 Operator : JU/SJ
 Sample : J2460-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MDP-B-1-18-20

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	493	498	508	rBV	80384	102812	4.26%	0.498%
2	5.422	563	567	581	rBV	2336937	2372904	98.33%	11.492%
3	6.445	736	741	755	rBV	2417354	2358449	97.73%	11.422%
4	6.575	759	763	766	rBV	2674374	2413133	100.00%	11.687%
5	6.804	798	802	805	rBV	892229	689079	28.56%	3.337%
6	6.957	824	828	832	rBV	1807851	1671750	69.28%	8.096%
7	7.369	894	898	901	rBV	1523922	1361933	56.44%	6.596%
8	7.610	935	939	941	rBV	48206	45219	1.87%	0.219%
9	7.987	1000	1003	1007	rBV	33986	34392	1.43%	0.167%
10	8.063	1013	1016	1017	rBV	41140	31270	1.30%	0.151%
11	8.087	1017	1020	1024	rVV	1023779	848940	35.18%	4.111%
12	8.140	1026	1029	1032	rVB3	40767	44485	1.84%	0.215%
13	8.375	1066	1069	1073	rBV4	42034	43055	1.78%	0.209%
14	8.675	1116	1120	1123	rBV	85222	73810	3.06%	0.357%
15	8.763	1132	1135	1139	rVB4	19438	26400	1.09%	0.128%
16	8.957	1165	1168	1172	rBV3	25511	40444	1.68%	0.196%
17	8.992	1172	1174	1178	rVB3	19614	27996	1.16%	0.136%
18	9.034	1178	1181	1185	rBV	28838	29993	1.24%	0.145%
19	9.075	1185	1188	1190	rBV	32825	28959	1.20%	0.140%
20	9.104	1190	1193	1196	rVB	63547	52430	2.17%	0.254%
21	9.163	1199	1203	1206	rBV	2197049	1772629	73.46%	8.585%
22	9.239	1213	1216	1219	rBV	126162	113665	4.71%	0.550%
23	9.492	1253	1259	1261	rBV4	19561	27716	1.15%	0.134%
24	9.557	1266	1270	1273	rBV	297548	282038	11.69%	1.366%
25	9.769	1303	1306	1310	rVB	100111	78915	3.27%	0.382%
26	9.845	1315	1319	1327	rVB	933200	856828	35.51%	4.150%
27	10.269	1388	1391	1394	rVB	74671	58914	2.44%	0.285%
28	10.486	1422	1428	1430	rBV	21626	26886	1.11%	0.130%
29	10.633	1450	1453	1465	rVV	1370055	1286138	53.30%	6.229%
30	10.739	1468	1471	1481	rVB	59964	63819	2.64%	0.309%
31	11.333	1568	1572	1584	rBV	831481	764209	31.67%	3.701%
32	12.727	1805	1809	1813	rBV	69490	63075	2.61%	0.305%
33	12.916	1837	1841	1845	rBV	1481810	1308338	54.22%	6.336%
34	13.398	1917	1923	1927	rBV5	21846	33068	1.37%	0.160%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.774	1980	1987	1990	rBV	124874	155668	6.45%	0.754%
36	13.810	1990	1993	2003	rVB2	82471	102999	4.27%	0.499%
37	13.974	2018	2021	2031	rVB	626063	642803	26.64%	3.113%
38	14.816	2161	2164	2169	rVB	213828	221730	9.19%	1.074%
39	15.445	2266	2271	2277	rBV	365223	491615	20.37%	2.381%

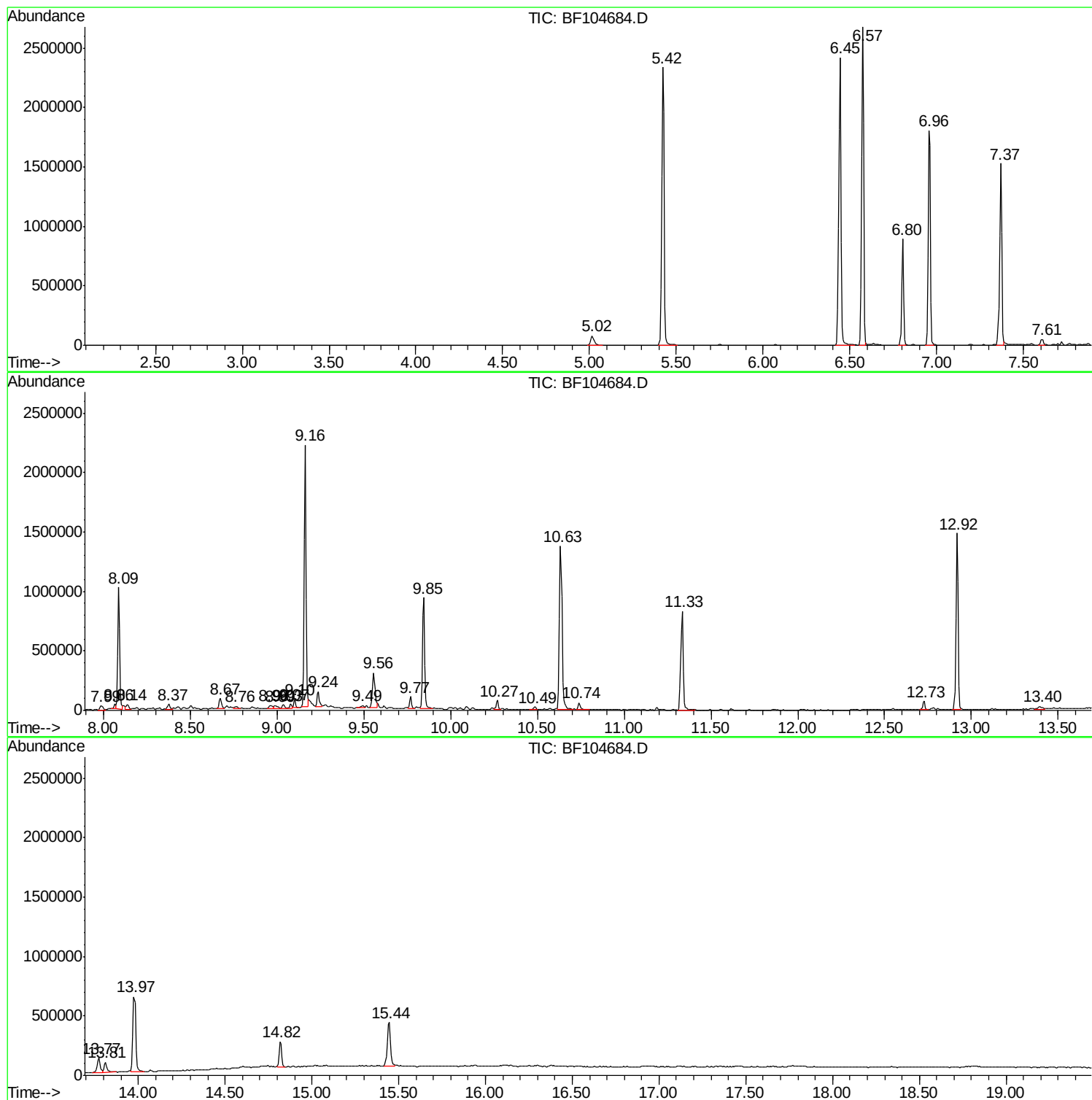
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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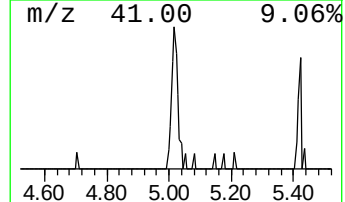
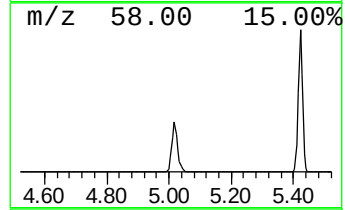
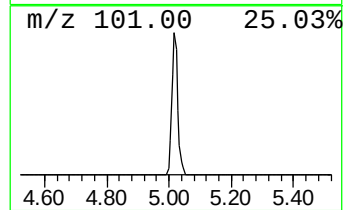
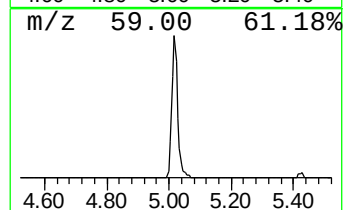
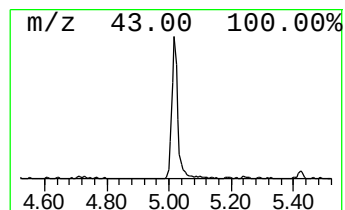
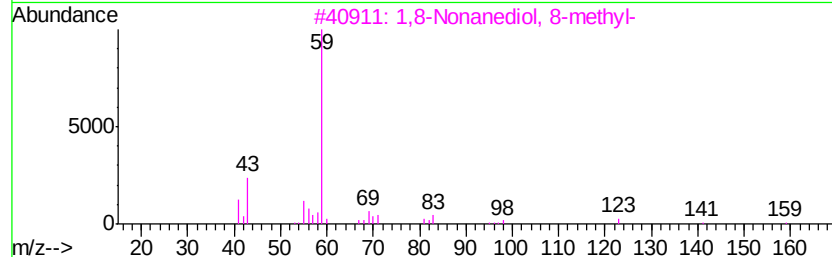
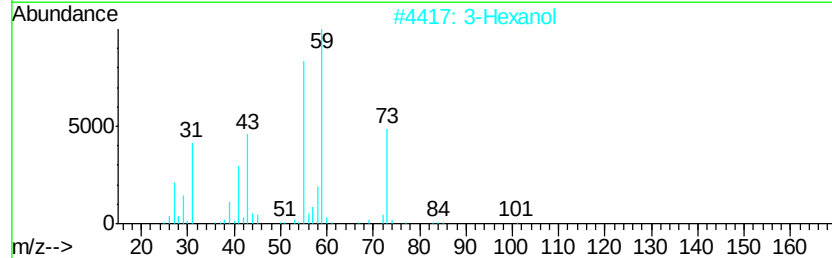
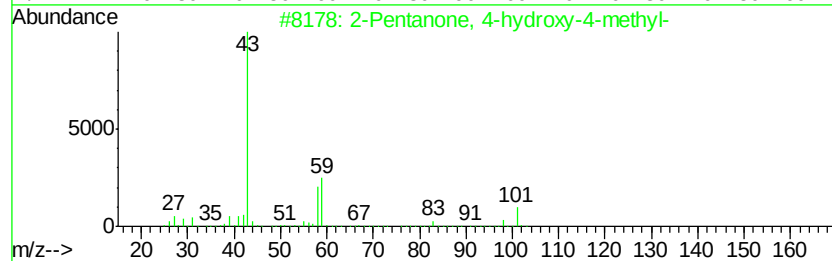
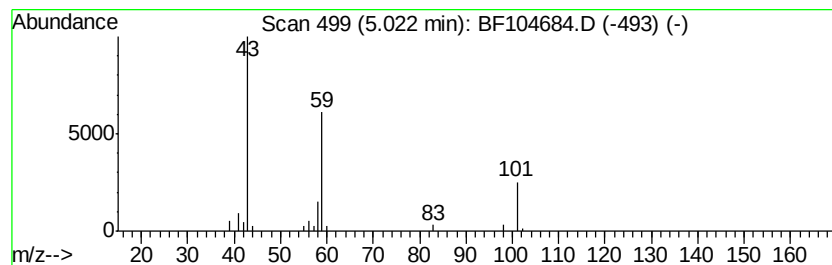
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	2.98 ng	102812	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		3-Hexanol	102	C6H14O	000623-37-0	28
3		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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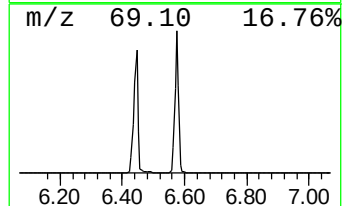
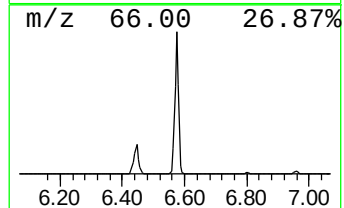
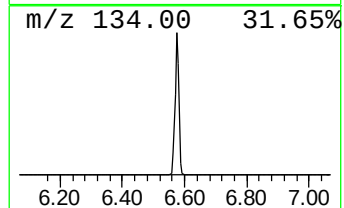
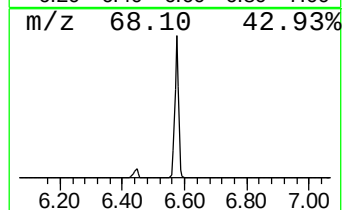
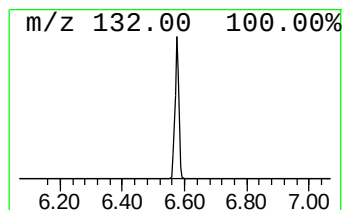
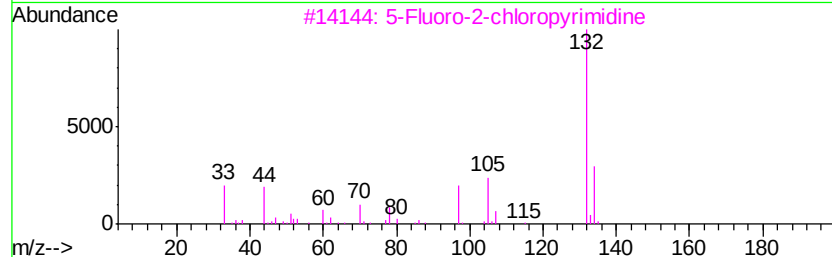
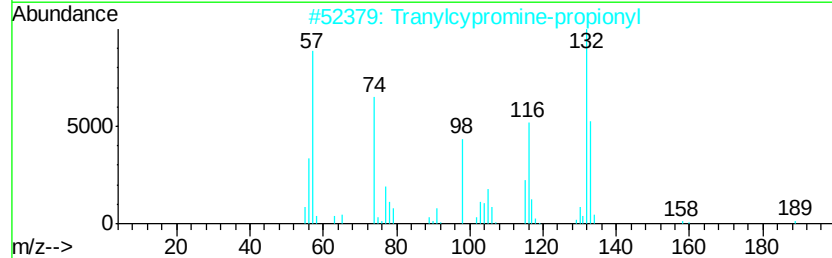
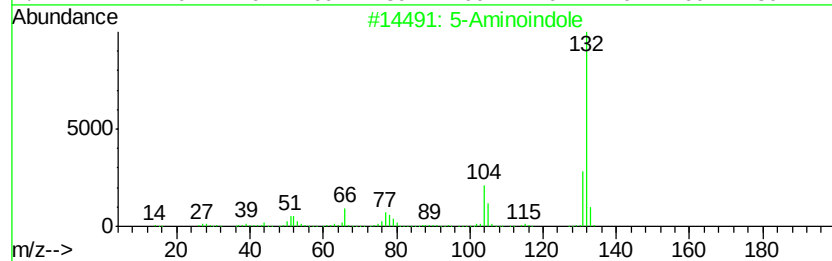
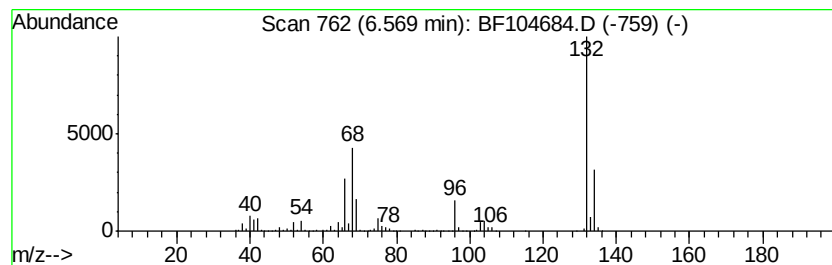
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	70.04 ng	2413130	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Aminoindole	132	C8H8N2	005192-03-0	12
2			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5			1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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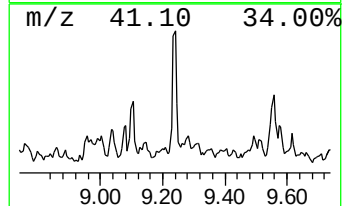
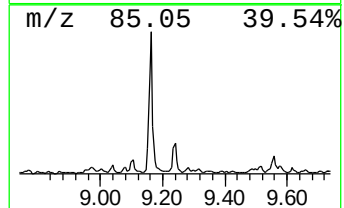
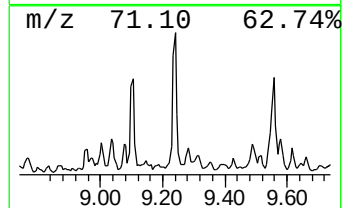
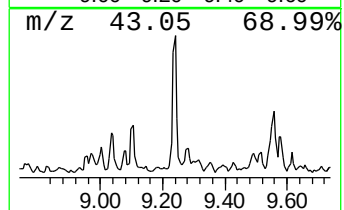
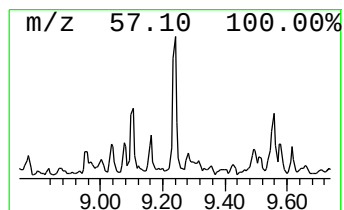
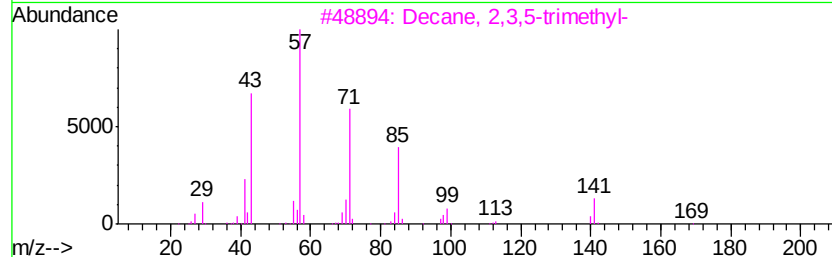
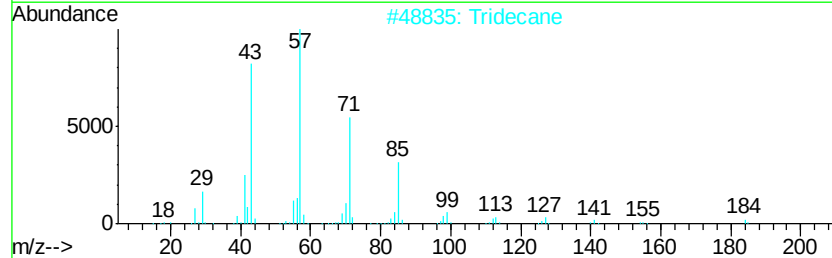
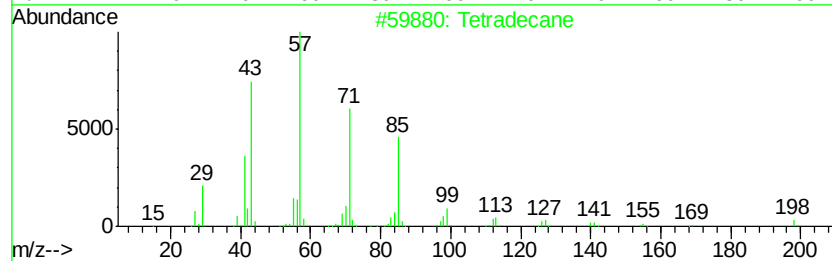
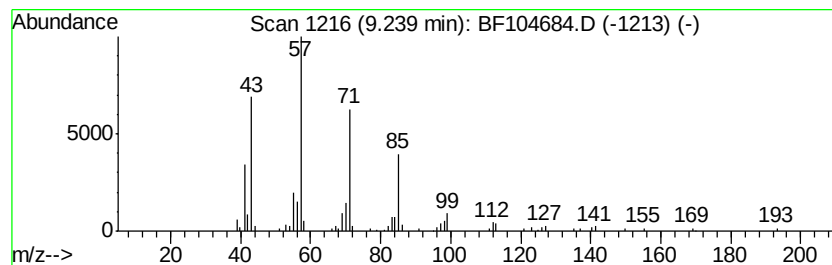
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Tetradecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.24	2.65 ng	113665	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetradecane	198	C14H30	000629-59-4	91
2		Tridecane	184	C13H28	000629-50-5	90
3		Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	90
4		Hexadecane	226	C16H34	000544-76-3	90
5		Dodecane	170	C12H26	000112-40-3	90



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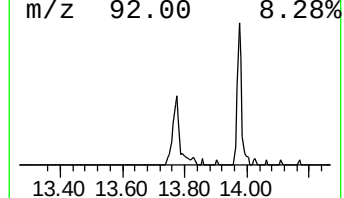
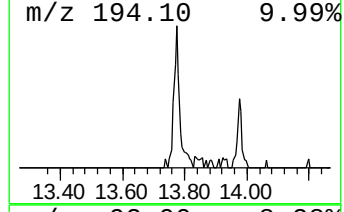
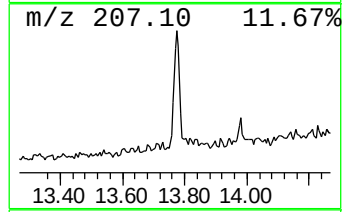
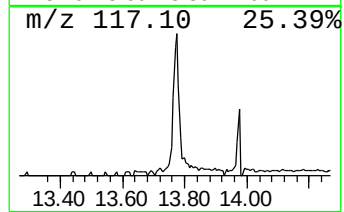
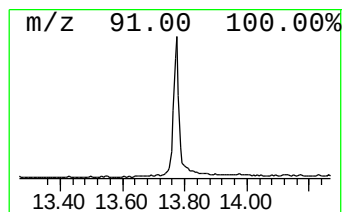
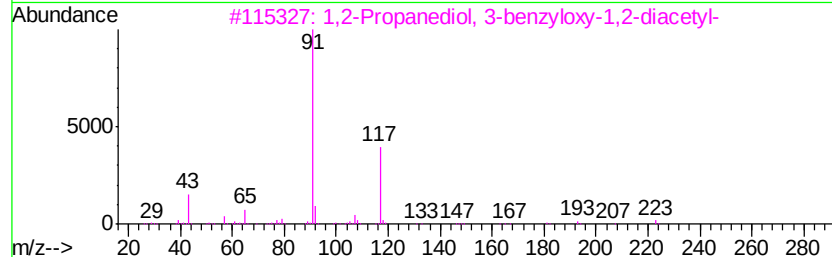
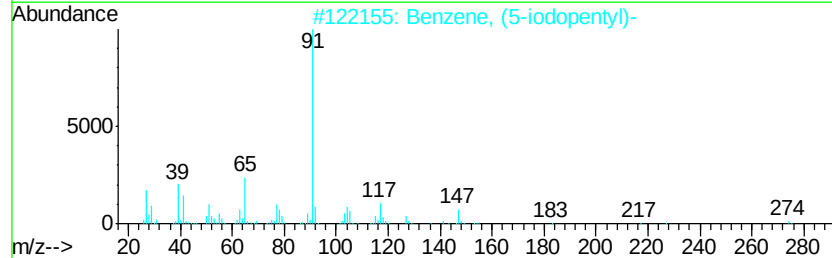
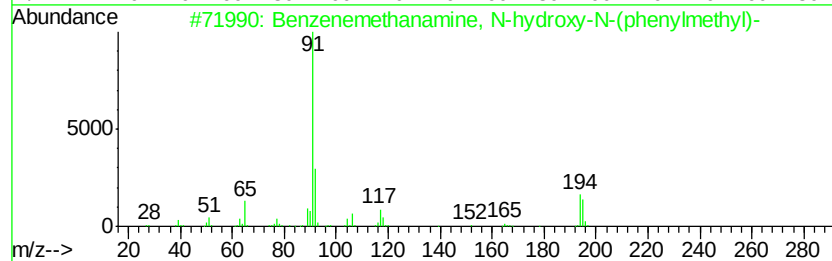
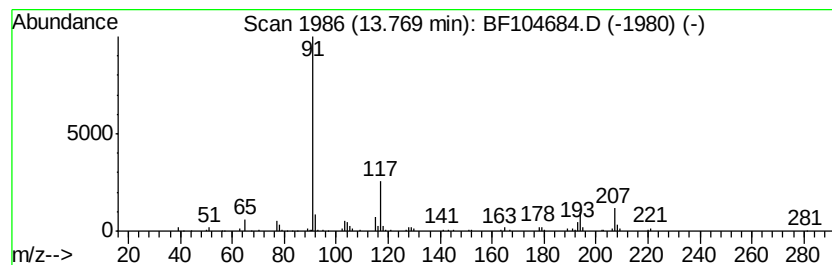
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown13.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	4.84 ng	155668	Chrysene-d12	13.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenemethanamine, N-hydroxy-N-...	213	C14H15NO	000621-07-8	23
2		Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	17
3		1,2-Propanediol, 3-benzoyloxy-1,2...	266	C14H18O5	013754-10-4	12
4		Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	10
5		2,3-Dihydrobenzoxazol-2-one-3-ca...	314	C15H10N2O6	300808-99-5	10



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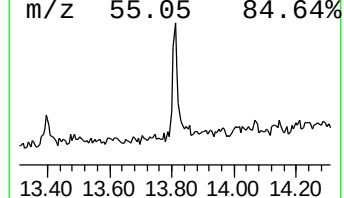
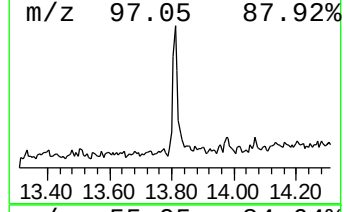
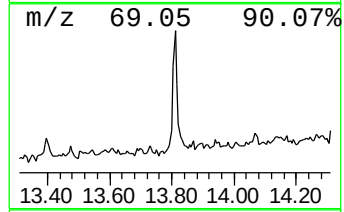
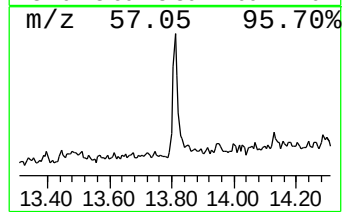
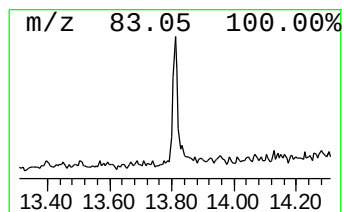
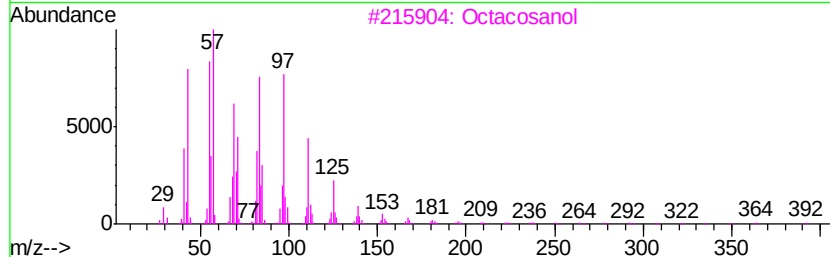
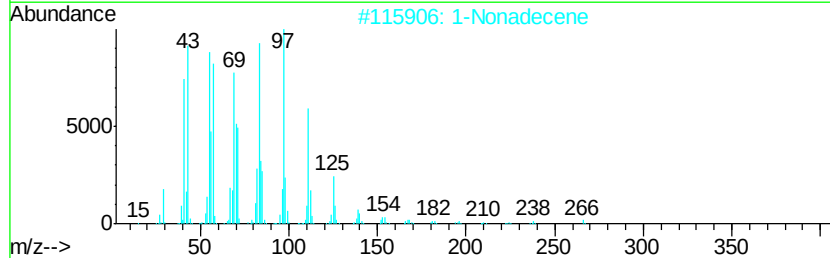
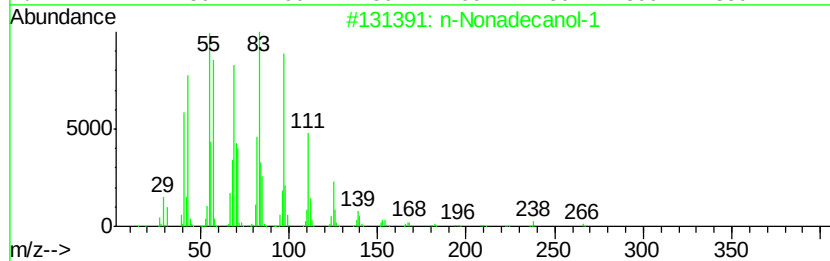
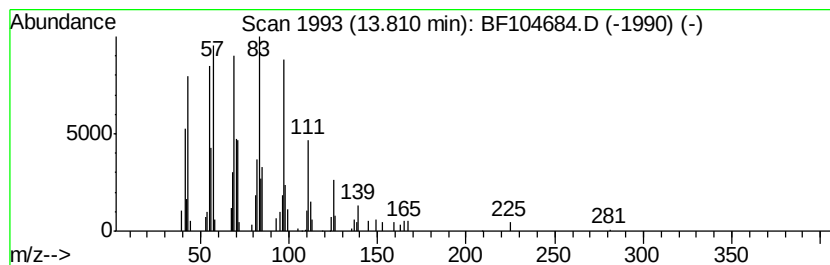
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	3.20 ng	102999	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Nonadecene	266	C19H38	018435-45-5	94
3	Octacosanol	410	C28H58O	000557-61-9	93
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
Data File : BF104684.D
Acq On : 20 Apr 2018 19:40
Operator : JU/SJ
Sample : J2460-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MDP-B-1-18-20

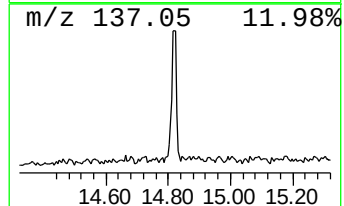
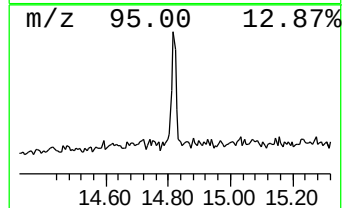
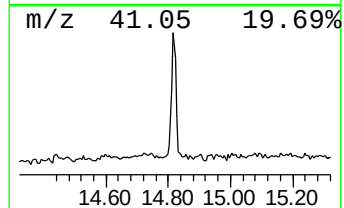
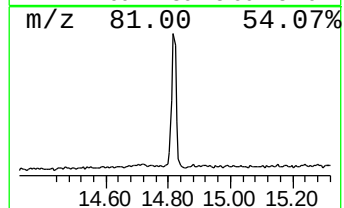
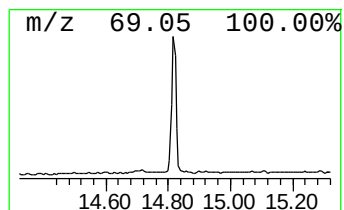
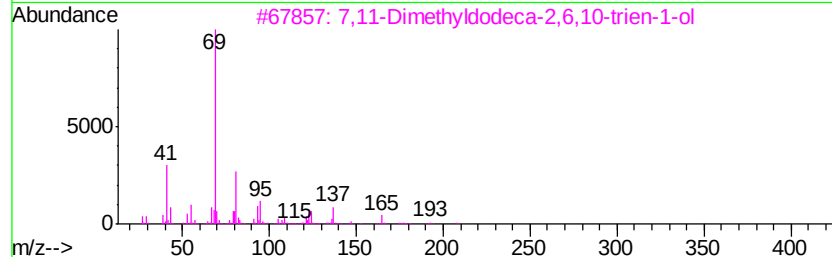
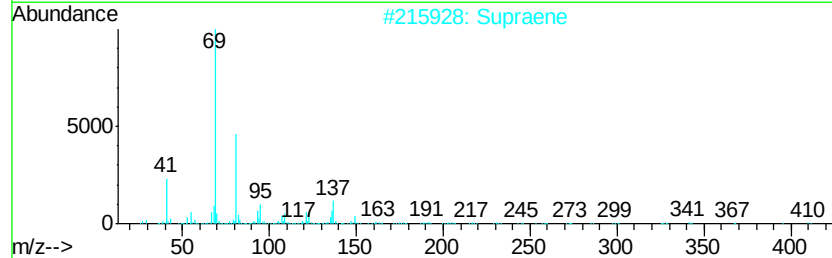
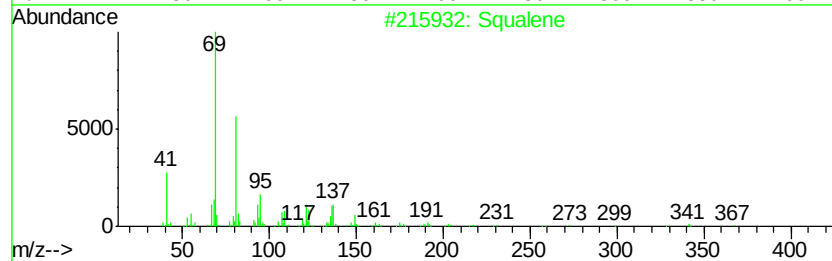
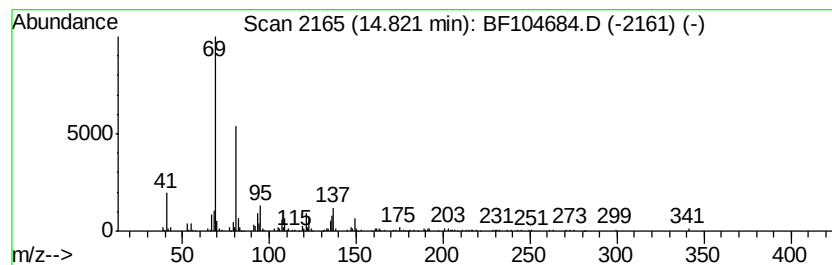
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	9.02 ng	221730	Perylene-d12	15.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	94
2		Supraene	410	C30H50	007683-64-9	91
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
4		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	80
5		1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	78



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042018\
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MDP-B-1-18-20

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	3.0	ng	102812	1	6.80	689079	20.0
unknown6.57	6.57	70.0	ng	2413130	1	6.80	689079	20.0
Tetradecane	9.24	2.6	ng	113665	3	9.85	856828	20.0
unknown13.77	13.77	4.8	ng	155668	5	13.97	642803	20.0
n-Nonadecanol-1	13.81	3.2	ng	102999	5	13.97	642803	20.0
Squalene	14.82	9.0	ng	221730	6	15.44	491615	20.0